Exploiting Sparsity in Bayesian Inverse Problems of Parametric Operator Equations

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Outline

1. Bayesian Inversion of Parametric Operator Equations
2. Sparsity of the Forward Solution
3. Sparsity of the Posterior
4. Sparse Quadrature
5. Numerical Results and Current Research Projects
   - Model Parametric Parabolic Problem
   - Model Parametric Elliptic Problem (Lognormal Prior)
   - Uncertainty Quantification in Nano Optics
   - High Dimensional Initial Value Problem
6. Summary
Inverse Problem

Physical Model

\[ G(u) \rightarrow \delta \]

- \( u \) parameter vector / parameter function
- \( G \) the forward map modelling the physical process
- \( \delta \) result / observations

Forward Problem

Find the output \( \delta \) for given parameters \( u \)

\[ \rightarrow \text{well-posed} \]

Inverse Problem

Find the parameters \( u \) from (noisy) observations \( \delta \)

\[ \rightarrow \text{ill-posed} \]
Inverse Problem

Find the unknown data $u \in X$ from noisy observations

$$\delta = G(u) + \eta,$$

- $u$ parameter vector / parameter function
- $G$ the forward map modelling the physical process
- $O$ bounded, linear observation operator
- $G$ uncertainty-to-observation map, $G = O \circ G$
- $\delta$ noisy observations
- $\eta$ observational noise
Inverse Problem

Find the unknown data $u \in X$ from noisy observations

$$\delta = G(u) + \eta,$$

Deterministic optimization problem

$$\min_u \frac{1}{2} \| \delta - G(u) \|^2 + R(u)$$

- $\| \delta - G(u) \|$ potential / data misfit
- $R$ regularization term
Inverse Problem

Find the unknown data \( u \in X \) from noisy observations

\[
\delta = \mathcal{G}(u) + \eta,
\]

Deterministic optimization problem

\[
\min_u \frac{1}{2} \| \delta - \mathcal{G}(u) \|^2 + R(u)
\]

- Large-scale, deterministic optimization problem
- No quantification of the uncertainty in the unknown \( u \)
- Proper choice of the regularization term \( R \)
Inverse Problem

Find the unknown data \( u \in X \) from noisy observations

\[
\delta = \mathcal{G}(u) + \eta,
\]

Bayesian inverse problem

\[
\delta = \mathcal{G}(u) + \eta
\]

- \( u, \eta, \delta \) random variables / fields
- Goal of computation: moments of system quantities under the posterior w.r. to noisy data \( \delta \)
Inverse Problem

Find the unknown data $u \in X$ from noisy observations

$$\delta = \mathcal{G}(u) + \eta,$$

Bayesian inverse problem
Inverse Problem

Find the unknown data $u \in X$ from noisy observations

$$\delta = G(u) + \eta,$$

Bayesian inverse problem
Inverse Problem

Find the unknown data $u \in X$ from noisy observations

$$\delta = \mathcal{G}(u) + \eta,$$

Bayesian inverse problem

$$\delta = \mathcal{G}(u) + \eta$$

- Quantification of uncertainty in $u$ and system quantities
- Well-posedness of the inverse problem
- Incorporation of prior knowledge on the uncertain data $u$
- Need of efficient approximations of the posterior
Bayesian Inverse Problems (Stuart 2010)

Find the unknown data \( u \in X \) from noisy observations

\[
\delta = \mathcal{G}(u) + \eta,
\]

Goal: Efficient estimation of system quantities from noisy observations

- Infinite-dimensional parameter space
- Fast convergence by exploiting sparsity of the underlying forward problem
- Suitable for application to a broad class of forward problems
Bayesian Inverse Problems (Stuart 2010)

Find the unknown data $u \in X$ from noisy observations

$$\delta = \mathcal{G}(u) + \eta,$$

**Goal: Efficient estimation of system quantities from noisy observations**

- Infinite-dimensional parameter space
- Fast convergence by exploiting sparsity of the underlying forward problem
- Suitable for application to a broad class of forward problems

UQ in Nano Optics
Bayesian Inverse Problems (Stuart 2010)

Find the unknown data \( u \in X \) from noisy observations

\[
\delta = \mathcal{G}(u) + \eta,
\]

Goal: Efficient estimation of system quantities from noisy observations

- Infinite-dimensional parameter space
- Fast convergence by exploiting sparsity of the underlying forward problem
- Suitable for application to a broad class of forward problems

UQ in Biochemical Networks

Source: Chen et al.
Bayesian Inverse Problems (Stuart 2010)

Find the unknown data \( u \in X \) from noisy observations

\[
\delta = G(u) + \eta,
\]

- \( X \) separable Banach space
- \( G : X \mapsto \mathcal{X} \) the forward map

Abstract Operator Equation

Given \( u \in X \), find \( q \in \mathcal{X} : \ A(u; q) = F(u) \) in \( \mathcal{Y}' \)

with \( A(u; \cdot) \in \mathcal{L} (\mathcal{X}, \mathcal{Y}') \), \( F : X \mapsto \mathcal{Y}' \), \( \mathcal{X}, \mathcal{Y} \) reflexive Banach spaces, \( a(v, w) := \langle w, Av \rangle_{\mathcal{Y}'} \) \( \forall v \in \mathcal{X}, w \in \mathcal{Y} \) corresponding bilinear form

- \( \mathcal{O} : \mathcal{X} \mapsto \mathbb{R}^K \) bounded, linear observation operator
- \( \mathcal{G} : X \mapsto \mathbb{R}^K \) uncertainty-to-observation map, \( \mathcal{G} = \mathcal{O} \circ G \)
- \( \eta \in \mathbb{R}^K \) the observational noise (\( \eta \sim \mathcal{N}(0, \Gamma) \))
Bayesian Inverse Problems (Stuart 2010)

Find the unknown data \( u \in X \) from noisy observations

\[
\delta = \mathcal{G}(u) + \eta,
\]

- \( X \) separable Banach space
- \( \mathcal{G} : X \mapsto \mathcal{X} \) the forward map
- \( \mathcal{O} : \mathcal{X} \mapsto \mathbb{R}^K \) bounded, linear observation operator
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- \( \eta \in \mathbb{R}^K \) the observational noise (\( \eta \sim \mathcal{N}(0, \Gamma) \))

Least squares potential \( \Phi : X \times \mathbb{R}^K \to \mathbb{R} \)

\[
\Phi(u; \delta) := \frac{1}{2} \left( (\delta - \mathcal{G}(u))^\top \Gamma^{-1} (\delta - \mathcal{G}(u)) \right)
\]

Reformulation of the forward problem with unknown stochastic input data as an infinite dimensional, parametric deterministic problem
Bayesian Inverse Problems (Stuart 2010)

Parametric representation of the unknown $u$

$$u = u(y) := \langle u \rangle + \sum_{j \in \mathbb{J}} y_j \psi_j \in X$$

- $y = (y_j)_{j \in \mathbb{J}}$ iid sequence of real-valued random variables $y_j \sim \mathcal{U}[-1, 1]$
- $\langle u \rangle, \psi_j \in X$
- $\mathbb{J}$ finite or countably infinite index set

Prior measure on the uncertain input data

$$\mu_0(dy) := \bigotimes_{j \in \mathbb{J}} \frac{1}{2} \lambda_1(dy_j).$$

- $(U, \mathcal{B}) = \left([-1, 1]^\mathbb{J}, \bigotimes_{j \in \mathbb{J}} \mathcal{B}^1[-1, 1]\right)$ measurable space
Bayesian Inverse Problem

Theorem (ChS and Stuart 2011)

Assume that \( G(u) \bigg|_{u=\langle u \rangle + \sum_{j \in J} y_j \psi_j} \) is bounded and continuous.

Then \( \mu^\delta(dy) \), the distribution of \( y \in U \) given \( \delta \), is absolutely continuous with respect to \( \mu_0(dy) \), and

\[
\frac{d\mu^\delta}{d\mu_0}(y) = \frac{1}{Z} \Theta(y)
\]

with the parametric Bayesian posterior \( \Theta \) given by

\[
\Theta(y) = \exp\left(-\Phi(u; \delta)\right) \bigg|_{u=\langle u \rangle + \sum_{j \in J} y_j \psi_j},
\]

and the normalization constant

\[
Z = \int_U \Theta(y) \mu_0(dy).
\]
Bayesian Inverse Problem

Expectation of a *Quantity of Interest* $\phi : X \rightarrow S$

$$\mathbb{E}^{\mu_\delta}[\phi(u)] = Z^{-1} \int_U \exp(-\Phi(u; \delta)) \phi(u) \bigg|_{u=\langle u \rangle + \sum_{j \in J} y_j \psi_j} \mu_0(dy) =: Z' / Z$$

with $Z = \mathbb{E}^{\mu_\delta}[1] = \int_U \exp(-\frac{1}{2} ((\delta - G(u))^	op \Gamma^{-1} (\delta - G(u)))) \mu_0(dy)$.

- Reformulation of the forward problem with unknown stochastic input data as an infinite dimensional, parametric deterministic problem
- Parametric, deterministic representation of the derivative of the posterior measure with respect to the prior $\mu_0$
- Approximation of $Z'$ and $Z$ to compute the expectation of QoI under the posterior given data $\delta$

**Efficient algorithm to approximate the conditional expectations given the data with dimension-independent rates of convergence**
Bayesian Inverse Problem

Expectation of a Quantity of Interest $\phi : X \rightarrow S$

$$\mathbb{E}^{\mu_0^\delta}[\phi(u)] = Z^{-1} \int_U \exp(-\Phi(u; \delta)) \phi(u) \bigg|_{u=\langle u \rangle + \sum_{j \in J} y_j \psi_j} \mu_0(dy) =: Z' / Z$$

with $Z = \mathbb{E}^{\mu_0^\delta}[1] = \int_U \exp\left(-\frac{1}{2} \left( (\delta - G(u))^\top \Gamma^{-1} (\delta - G(u)) \right) \right) \mu_0(dy)$.

Exploiting sparsity in the parametric operator equation

- Parameters belonging to a specified sparsity class
- Analytic regularity of the parametric, deterministic Bayesian posterior
- Parametric, deterministic Bayesian posterior belongs to the same sparsity class

→ Sparsity of Legendre pce + dimension-independent convergence rates for Smolyak integration algorithms
$(b, p, \epsilon)$-Analyticity

$(b, p, \epsilon) : 1$ (well-posedness)

For each $y \in U$, there exists a unique realization $u(y) \in X$ and a unique solution $q(y) \in \mathcal{X}$ of the forward problem. This solution satisfies the a-priori estimate

$$\forall y \in U : \quad \|q(y)\|_X \leq C_0.$$ 

$(b, p, \epsilon) : 2$ (analyticity)

There exist $0 < p < 1$ and $b = (b_j)_{j \in J} \in \ell^p(J)$ such that for $\epsilon > 0$, there exist $C_\epsilon > 0$ and $\rho = (\rho_j)_{j \in J}$ of poly-radii $\rho_j > 1$ such that

$$\sum_{j \in J} (\rho_j - 1)b_j \leq \epsilon,$$

and $U \ni y \mapsto q(y) \in \mathcal{X}$ admits an analytic continuation to the open polyellipse $\mathcal{E}_\rho := \prod_{j \in J} \mathcal{E}_{\rho_j} \subset \mathbb{C}^J$ with

$$\forall z \in \mathcal{E}_\rho : \quad \|q(z)\|_X \leq C_\epsilon.$$
$(b, p, \epsilon)$-Analyticity of Parametric Operator Families

$u \in X : A(u; q) = F(u) \quad q \in \mathcal{X}$

Assumption A1

For $\epsilon > 0$ and some $0 < p < 1$, there exists a positive sequence $b = (b_j)_{j \geq 1} \in \ell^p(\mathbb{N})$, such that for any sequence $\rho := (\rho_j)_{j \geq 1}$ with $\rho_j > 1$, $\sum_{j \in \mathbb{J}} (\rho_j - 1) b_j \leq \epsilon$, $a$ and $F$ are holomorphic in $\mathcal{E}_\rho$.

Assumption A2

The holomorphic extensions satisfy the uniform continuity conditions

$$\sup_{w \in \mathcal{Y} \setminus \{0\}} \frac{|f(z; w)|}{\|w\|_\mathcal{Y}} \leq M, \quad \sup_{v \in \mathcal{X} \setminus \{0\}, w \in \mathcal{Y} \setminus \{0\}} \frac{|a(z; v, w)|}{\|v\|_\mathcal{X} \cdot \|w\|_\mathcal{Y}} \leq R,$$

with $M < \infty$, $f$ corresponding linear form of $F$.

Assumption A3

There hold the uniform inf-sup conditions:

$$\inf_{v \in \mathcal{X} \setminus \{0\}} \sup_{w \in \mathcal{Y} \setminus \{0\}} \frac{|a(z; v, w)|}{\|v\|_\mathcal{X} \cdot \|w\|_\mathcal{Y}} \geq r \quad \text{and} \quad \inf_{w \in \mathcal{Y} \setminus \{0\}} \sup_{v \in \mathcal{X} \setminus \{0\}} \frac{|a(z; v, w)|}{\|v\|_\mathcal{X} \cdot \|w\|_\mathcal{Y}} \geq r$$

with $0 < r \leq R < \infty$. 
(b, p, ϵ)-Analyticity of Parametric Operator Families

\[ u \in X : A(u; q) = F(u) \quad q \in \mathcal{X} \]

**Assumption A1** \( \alpha \) and \( F \) holomorphic in \( \mathcal{E}_\rho \)

**Assumption A2**

\[
\sup_{w \in \mathcal{Y} \setminus \{0\}} \frac{|f(z; w)|}{\|w\|_{\mathcal{Y}}} \leq M, \quad \sup_{v \in \mathcal{X} \setminus \{0\}, w \in \mathcal{Y} \setminus \{0\}} \frac{|a(z; v, w)|}{\|v\|_{\mathcal{X}} \|w\|_{\mathcal{Y}}} \leq R
\]

**Assumption A3**

\[
\inf_{v \in \mathcal{X} \setminus \{0\}} \sup_{w \in \mathcal{Y} \setminus \{0\}} \frac{|a(z; v, w)|}{\|v\|_{\mathcal{X}} \|w\|_{\mathcal{Y}}} \geq r \quad \text{und} \quad \inf_{w \in \mathcal{Y} \setminus \{0\}} \sup_{v \in \mathcal{X} \setminus \{0\}} \frac{|a(z; v, w)|}{\|v\|_{\mathcal{X}} \|w\|_{\mathcal{Y}}} \geq r
\]

**Theorem (Cohen, Chkifa, ChS 2013)**

Unter Assumptions **A1 - A3**, \( A(u; q) = A(u; q) - F(u) \) satisfies the \( (b, p, \epsilon) \)-holomorphy assumptions.
Theorem (Chkifa, Cohen, DeVore and ChS)

Assume that the parametric forward solution map $q(y)$ admits a $(b, p, \epsilon)$-analytic extension to the poly-ellipse $\mathcal{E}_\rho \subset \mathbb{C}^J$.

- The Legendre series converges unconditionally,

$$q(y) = \sum_{\nu \in \mathcal{F}} q^P_{\nu} P_\nu(y) \quad \text{in } L^\infty(U, \mu_0; \mathcal{X})$$

with Legendre polynomials $P_k(1) = 1$, $\|P_k\|_{L^\infty(-1,1)} = 1$, $k = 0, 1, \ldots$.

- There exists a $p$-summable, monotone envelope $q = \{q_{\nu}\}_{\nu \in \mathcal{F}}$, i.e. $q_{\nu} := \sup_{\mu \geq \nu} \|q^P_{\nu}\|_{\mathcal{X}}$ with $C(p, q) := \|q\|_{\ell^p(\mathcal{F})} < \infty$.

and monotone $\Lambda^P_N \subset \mathcal{F}$ corresponding to the $N$ largest terms of $q$ with

$$\sup_{y \in U} \left\| q(y) - \sum_{\nu \in \Lambda^P_N} q^P_{\nu} P_\nu(y) \right\|_{\mathcal{X}} \leq C(p, q) N^{-\left(1/p - 1\right)}.$$
Theorem (ClS and ChS 2013)

Assume that the forward solution map \( U \ni y \mapsto q(y) \) is \((b, p, \epsilon)\)-analytic for some \( 0 < p < 1 \).

Then the Bayesian posterior \( \Theta(y) \) is, as a function of the parameter \( y \), likewise \((b, p, \epsilon)\)-analytic, with the same \( p \) and the same \( \epsilon \).

Sketch of proof

- Establish holomorphy of the complex extension \( \Theta \) on the poly-ellipse \( \mathcal{E}_\rho \subset \mathbb{C}^J \)
- Derive bounds on the modulus of the posterior

\[
\sup_{z \in \mathcal{E}_\rho} |\Theta(z)| \leq \exp \left( \sup_{z \in \mathcal{E}_\rho} \frac{1}{2} \text{Im} \left( \mathcal{G}(u(z)) \right)^\top \Gamma^{-1} \text{Im} \left( \mathcal{G}(u(z)) \right) \right)
\]
Sparsity of the Posterior

Theorem (CLS and ChS 2013)

Assume that the forward solution map $U \ni y \mapsto q(y)$ is $(b, p, \epsilon)$–analytic for some $0 < p < 1$.

Then the Bayesian posterior $\Theta(y)$ is, as a function of the parameter $y$, likewise $(b, p, \epsilon)$–analytic, with the same $p$ and the same $\epsilon$.

N-term Approximation Results

$$\sup_{y \in U} \left\| \Theta(y) - \sum_{\nu \in \Lambda_N^P} \Theta^P \nu \nu(y) \right\|_{\mathcal{X}} \leq N^{-s} \left\| \theta^P \right\|_{\ell^p_m(F)}, \quad s := \frac{1}{p} - 1.$$  

Adaptive Smolyak quadrature algorithm with convergence rates depending only on the summability of the parametric operator.
Theorem (ClS and ChS 2013)

Assume that the forward solution map $U \ni y \mapsto q(y)$ is $(b, p, \epsilon)$–analytic for some $0 < p < 1$.

Then the Bayesian posterior $\Theta(y)$ is, as a function of the parameter $y$, likewise $(b, p, \epsilon)$–analytic, with the same $p$ and the same $\epsilon$.

Examples

- Parametric initial value ODEs (Hansen & ChS; Vietnam J. Math. 2013)
- Affine-parametric, linear operator equations (ClS & ChS; 2013)
- Semilinear elliptic PDEs (Hansen & ChS; Math. Nachr. 2013)
- Elliptic multiscale problems (Hoang & ChS; Analysis and Applications 2012)
- Nonaffine holomorphic-parametric, nonlinear problems (Cohen, Chkifa & ChS; 2013)
Univariate Quadrature

Univariate quadrature operators of the form

\[
Q^k(g) = \sum_{i=0}^{n_k} w^k_i \cdot g(z^k_i)
\]

with \( g : [-1, 1] \rightarrow \mathbb{R} \).

- \((Q^k)_{k \geq 0}\) sequence of univariate quadrature formulas
- \((z^k_j)_{j=0}^{n_k} \subset [-1, 1]\) with \( z^k_j \in [-1, 1], \forall j, k \) and \( z^k_0 = 0, \forall k \) quadrature points
- \( w^k_j, 0 \leq j \leq n_k, \forall k \in \mathbb{N}_0 \) quadrature weights

Assumption

(i) \((I - Q^k)(g_k) = 0, \forall g_k \in \mathbb{P}_k = \text{span}\{y^j : j \in \mathbb{N}_0, j \leq k\}\)

with \( I(g_k) = \int_{[-1,1]} g_k(y)\lambda_1(dy) \)

(ii) \( w^k_j > 0, \quad 0 \leq j \leq n_k, \forall k \in \mathbb{N}_0. \)
Univariate Quadrature

Univariate quadrature operators of the form

\[ Q^k(g) = \sum_{i=0}^{n_k} w_i^k \cdot g(z_i^k) \]

with \( g : [-1, 1] \rightarrow \mathbb{R} \).

- \((Q^k)_{k \geq 0}\) sequence of univariate quadrature formulas
- \((z_j^k)_{j=0}^{n_k} \subset [-1, 1] \) with \( z_j^k \in [-1, 1] \), \( \forall j, k \) and \( z_0^k = 0 \), \( \forall k \) quadrature points
- \( w_j^k \), \( 0 \leq j \leq n_k \), \( \forall k \in \mathbb{N}_0 \) quadrature weights

Univariate quadrature difference operator

\[ \Delta_j = Q^j - Q^{j-1}, \quad j \geq 0 \]

with \( Q^{-1} = 0 \) and \( z_0^0 = 0 \), \( w_0^0 = 1 \).
Univariate Quadrature

Univariate quadrature operators of the form

\[ Q^k(g) = \sum_{i=0}^{n_k} w^k_i \cdot g(z^k_i) \]

with \( g : [-1, 1] \mapsto \mathbb{R} \).

- \( (Q^k)_{k \geq 0} \) sequence of univariate quadrature formulas
- \( (z^k_j)_{j=0}^{n_k} \subset [-1, 1] \) with \( z^k_j \in [-1, 1], \forall j, k \) and \( z^k_0 = 0, \forall k \) quadrature points
- \( w^k_j, 0 \leq j \leq n_k, \forall k \in \mathbb{N}_0 \) quadrature weights

Univariate quadrature operator rewritten as telescoping sum

\[ Q^k = \sum_{j=0}^{k} \Delta_j \]

with \( \mathcal{Z}^k = \{ z^k_j : 0 \leq j \leq n_k \} \subset [-1, 1] \) set of points corresponding to \( Q^k \).
Sparse Quadrature Operator

Tensorized multivariate operators

\[ Q_\nu = \bigotimes_{j \geq 1} Q_{\nu_j}, \quad \Delta_\nu = \bigotimes_{j \geq 1} \Delta_{\nu_j} \]

with associated set of multivariate points \( Z_\nu = \times_{j \geq 1} Z_{\nu_j} \in U \).

- If \( \nu = 0_F \), then \( \Delta_\nu g = Q_\nu g = g(z_{0_F}) = g(0_F) \)
- If \( 0_F \neq \nu \in F \), with \( \hat{\nu} = (\nu_j)_{j \neq i} \)

\[ Q_\nu g = Q_{\nu_i} (t \mapsto \bigotimes_{j \geq 1} Q_{\hat{\nu}_j} g_t), \quad i \in I_\nu \]

and

\[ \Delta_\nu g = \Delta_{\nu_i} (t \mapsto \bigotimes_{j \geq 1} \Delta_{\hat{\nu}_j} g_t), \quad i \in I_\nu, \]

for \( g \in Z \), \( g_t \) is the function defined on \( Z^N \) by

\[ g_t(\hat{y}) = g(y), y = (\ldots, y_{i-1}, t, y_{i+1}, \ldots), i > 1 \text{ and } y = (t, y_2, \ldots), i = 1 \]
Sparse Quadrature Operator

For any finite monotone set $\Lambda \subseteq \mathcal{F}$, the quadrature operator is defined by

$$Q_\Lambda = \sum_{\nu \in \Lambda} \Delta_\nu = \sum_{\nu \in \Lambda} \bigotimes_{j \geq 1} \Delta_{\nu_j}$$

with associated collocation grid

$$\mathcal{Z}_\Lambda = \bigcup_{\nu \in \Lambda} \mathcal{Z}_\nu.$$
Sparse Quadrature Operator

For any finite monotone set $\Lambda \subset \mathcal{F}$, the quadrature operator is defined by

$$Q_{\Lambda} = \sum_{\nu \in \Lambda} \Delta_{\nu} = \sum_{\nu \in \Lambda} \bigotimes_{j \geq 1} \Delta_{\nu_j}$$

with associated collocation grid

$$\mathcal{Z}_{\Lambda} = \bigcup_{\nu \in \Lambda} \mathcal{Z}_{\nu}.$$
Convergence Rates for Adaptive Smolyak Integration

**Theorem**

Assume that the forward solution map \( U \ni y \mapsto q(y) \) is \((b, p, \epsilon)\)-analytic for some \( 0 < p < 1 \).

Then there exists a sequence \((\Lambda_N)_{N \geq 1}\) of monotone index sets \( \Lambda_N \subset \mathcal{F} \) such that \( \# \Lambda_N \leq N \) and

\[
|I[\Theta] - Q_{\Lambda_N}[\Theta]| \leq C^1 N^{-s},
\]

with \( s = 1/p - 1 \), \( I[\Theta] = \int_U \Theta(y) \mu_0(dy) \) and,

\[
\|I[\Psi] - Q_{\Lambda_N}[\Psi]\|_{\mathcal{X}} \leq C^2 N^{-s}, \quad s = \frac{1}{p} - 1.
\]

with \( I[\Psi] = \int_U \Psi(y) \mu_0(dy) \), \( C^1, C^2 > 0 \) independent of \( N \).

**Remark:** SAME index sets \( \Lambda_N \) for BOTH, \( Z' \) and \( Z \).

CIS and ChS Sparsity in Bayesian Inversion of Parametric Operator Equations, 2013.
Convergence Rates for Adaptive Smolyak Integration

Sketch of proof

- Relating the quadrature error with the Legendre coefficients

\[ |I(\Theta) - Q_\Lambda(\Theta)| \leq 2 \cdot \sum_{\nu \notin \Lambda} \gamma_\nu |\theta^P_\nu| \]

and

\[ \|I(\Psi) - Q_\Lambda(\Psi)\|_X \leq 2 \cdot \sum_{\nu \notin \Lambda} \gamma_\nu \|\psi^P_\nu\|_X \]

for any monotone set \( \Lambda \subset \mathcal{F} \), where \( \gamma_\nu := \prod_{j \in \mathcal{J}} (1 + \nu_j)^2. \)

- \( (\gamma_\nu |\theta^P_\nu|)_{\nu \in \mathcal{F}} \in l^p_m(\mathcal{F}) \) and \( (\gamma_\nu \|\psi^P_\nu\|_X)_{\nu \in \mathcal{F}} \in l^p_m(\mathcal{F}). \)

\[ \Rightarrow \exists \text{ sequence } (\Lambda_N)_{N \geq 1} \text{ of monotone sets } \Lambda_N \subset \mathcal{F}, \# \Lambda_N \leq N, \text{ such that the Smolyak quadrature converges with order } 1/p - 1. \]
Adaptive Construction of the Monotone Index Set

Successive identification of the $N$ largest contributions

$$|\Delta_\nu(\Theta)| = |\bigotimes_{j \geq 1} \Delta_{\nu_j}(\Theta)|, \quad \nu \in \mathcal{F}$$
Adaptive Construction of the Monotone Index Set

Successive identification of the $N$ largest contributions

$$\left| \Delta_\nu(\Theta) \right| = \left| \bigotimes_{j \geq 1} \Delta_{\nu_j}(\Theta) \right|, \quad \nu \in \mathcal{F}$$
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$$|\Delta_\nu(\Theta)| = \left| \bigotimes_{j \geq 1} \Delta_{\nu_j}(\Theta) \right|, \quad \nu \in \mathcal{F}$$

→ A. Chkifa, A. Cohen and ChS. High-dimensional adaptive sparse polynomial interpolation and applications to parametric PDEs, 2012.

Reduced set of neighbors

$$\mathcal{N}(\Lambda) := \{ \nu \notin \Lambda : \nu - e_j \in \Lambda, \forall j \in \mathbb{I}_\nu \text{ and } \nu_j = 0, \forall j > j(\Lambda) + 1 \}$$

with $j(\Lambda) = \max\{j : \nu_j > 0 \text{ for some } \nu \in \Lambda\}$, $\mathbb{I}_\nu = \{j \in \mathbb{N} : \nu_j \neq 0\} \subset \mathbb{N}$. 
Adaptive Construction of the Monotone Index Set

1: function ASG
2: Set $\Lambda_1 = \{0\}$, $k = 1$ and compute $\Delta_0(\Theta)$. 
3: Determine the reduced set of neighbors $\mathcal{N}(\Lambda_1)$. 
4: Compute $\Delta_\nu(\Theta)$, $\forall \nu \in \mathcal{N}(\Lambda_1)$. 
5: while $\sum_{\nu \in \mathcal{N}(\Lambda_k)} |\Delta_\nu(\Theta)| > tol$ do 
6: Select $\nu \in \mathcal{N}(\Lambda_k)$ with largest $|\Delta_\nu|$ and set $\Lambda_{k+1} = \Lambda_k \cup \{\nu\}$. 
7: Determine the reduced set of neighbors $\mathcal{N}(\Lambda_{k+1})$. 
8: Compute $\Delta_\nu(\Theta)$, $\forall \nu \in \mathcal{N}(\Lambda_{k+1})$. 
9: Set $k = k + 1$. 
10: end while 
11: end function

Numerical Experiments

Model parametric parabolic problem

\[
\frac{\partial}{\partial t} q(t, x) - \text{div}(u(x) \nabla q(t, x)) = 100 \cdot tx \\
q(0, x) = 0 \\
q(t, 0) = q(t, 1) = 0
\]

\((t, x) \in T \times D\), \(x \in D\), \(t \in T\)

with

\[
\begin{align*}
    u(x, y) &= \langle u \rangle + \sum_{j=1}^{64} y_j \psi_j, \text{where } \langle u \rangle = 1 \text{ and } \psi_j = \alpha_j \chi_{D_j}
    
\end{align*}
\]

where

\[
D_j = [(j - 1) \frac{1}{64}, j \frac{1}{64}], \quad y = (y_j)_{j=1,...,64} \quad \text{and} \quad \alpha_j = \frac{0.9}{j^\zeta}, \quad \zeta = 2, 3, 4.
\]

- Finite element method using continuous, piecewise linear ansatz functions in space, backward Euler scheme in time
- Uniform mesh with meshwidth \(h_T = h_D = 2^{-11}\)
- LAPACK’s DPTSV routine
Numerical Experiments

Find the unknown data $u$ for given (noisy) data $\delta$,

$$\delta = \mathcal{G}(u) + \eta,$$

Expectation of interest $Z'/Z$

$$Z' = \int_U \exp(-\Phi(u; \delta)) \phi(u) \bigg|_{u = \langle u \rangle + \sum_{j=1}^{64} y_j \psi_j} \mu_0(dy)$$

$$Z = \int_U \exp(-\Phi(u; \delta)) \bigg|_{u = \langle u \rangle + \sum_{j=1}^{64} y_j \psi_j} \mu_0(dy)$$

- Observation operator $\mathcal{O}$ consists of system responses at $K$ observation points in $T \times D$ at $t_i = \frac{i}{2^{N_K,T}}, i = 1, \ldots, 2^{N_K,T} - 1$, $x_j = \frac{j}{2^{N_K,D}}, k = 1, \ldots, 2^{N_K,D} - 1$, $o_k(\cdot, \cdot) = \delta(\cdot - t_k)\delta(\cdot - x_k)$ with $K = 3$, $N_{K,D} = 2$, $N_{K,T} = 1$
- $\mathcal{G} : X \rightarrow \mathbb{R}^K$, with $\phi(u) = G(u)$
- $\eta = (\eta_j)_{j=1,\ldots,K}$ iid with $\eta_j \sim \mathcal{N}(0, 1)$
Numerical Experiments

Quadrature points

- **Clenshaw-Curtis (CC)**

\[ z_j^k = -cos \left( \frac{\pi j}{n_k - 1} \right) \quad j = 0, \ldots, n_k - 1, \text{ if } n_k > 1 \text{ and} \]

\[ z_0^k = 0, \text{ if } n_k = 1 \]

with \( n_0 = 1 \) and \( n_k = 2^k + 1, \text{ for } k \geq 1 \)

- **R-Leja sequence (RL)**
Numerical Experiments

Quadrature points

- Clenshaw-Curtis (CC)
- \( \mathfrak{H} \)-Leja sequence (RL)

projection on \([-1, 1]\) of a Leja sequence for the complex unit disk initiated at \(i\)

\[
\begin{align*}
z_0^k &= 0, z_1^k = 1, z_2^k = -1, \text{ if } j = 0, 1, 2 \text{ and } \\
z_j^k &= \mathfrak{H}(\hat{z}), \text{ with } \hat{z} = \arg\max_{|z| \leq 1} \prod_{l=1}^{j-1} |z - z_l^k|, \text{ if } j \text{ odd, } \\
z_j^k &= -z_{j-1}^k, \text{ if } j \text{ even, }
\end{align*}
\]

with \(n_k = 2 \cdot k + 1, \text{ for } k \geq 0\)


Figure: Comparison of the estimated error and actual error. Plots of error w.r. to reference solutions of the normalization constant $Z$ w.r. to the cardinality of the index set $\Lambda_N$ (l.) and w.r. to the PDE solves needed (r.) based on the sequence CC with $K = 3$, $\eta \sim \mathcal{N}(0, 1)$ and with $\zeta = 2, 3, 4$, $h_T = h_D = 2^{-11}$ for the reference and the adaptively computed solution.
Figure: Comparison of the estimated error and actual error. Plots of error w.r. to reference solutions of the normalization constant $Z$ w.r. to the cardinality of the index set $\Lambda_N$ (l.) and w.r. to the PDE solves needed (r.) based on the sequence RL with $K = 3$, $\eta \sim \mathcal{N}(0, 1)$ and with $\zeta = 2, 3, 4$, $h_T = h_D = 2^{-11}$ for the reference and the adaptively computed solution.
Figure: Comparison of the estimated error and actual error. Plots of error w.r. to reference solutions of the quantity $Z'$ w.r. to the cardinality of the index set $\Lambda_N$ (l.) and w.r. to the PDE solves needed (r.) based on the sequence CC with $K = 3$, $\eta \sim \mathcal{N}(0, 1)$ and with $\zeta = 2, 3, 4$, $h_T = h_D = 2^{-11}$ for the reference and the adaptively computed solution.
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Numerical Experiments

Model parametric parabolic problem

\[ \partial_t q(t, x) - \text{div}(u(x)\nabla q(t, x)) = 100 \cdot tx \quad (t, x) \in T \times D, \]
\[ q(0, x) = 0 \quad x \in D, \]
\[ q(t, 0) = q(t, 1) = 0 \quad t \in T \]

with

\[ u(x, y) = \langle u \rangle + \sum_{j=1}^{128} y_j \psi_j \text{, where } \langle u \rangle = 1 \text{ and } \psi_j = \alpha_j \chi_{D_j} \]

where \( D_j = [(j - 1) \frac{1}{128}, j \frac{1}{128}] \), \( y = (y_j)_{j=1,...,128} \) and \( \alpha_j = \frac{0.6}{j^\zeta} \), \( \zeta = 2, 3, 4 \).

- Finite element method using continuous, piecewise linear ansatz functions in space, backward Euler scheme in time
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Figure: Comparison of the estimated error and actual error. Plots of error w.r. to reference solutions of the normalization constant $Z$ w.r. to the cardinality of the index set $\Lambda_N$ (l.) and w.r. to the PDE solves needed (r.) based on the sequence CC with $K = 3$, $\eta \sim \mathcal{N}(0, 1)$ and with $\zeta = 2, 3, 4$, $h_T = h_D = 2^{-11}$ for the reference and the adaptively computed solution.
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Quantity $Z'$ (128 parameters)

![Graphs showing comparison of estimated and actual errors](image)

**Figure**: Comparison of the estimated error and actual error. Plots of error w.r. to reference solutions of the quantity $Z'$ w.r. to the cardinality of the index set $\Lambda_N$ (l.) and w.r. to the PDE solves needed (r.) based on the sequence CC with $K = 3$, $\eta \sim \mathcal{N}(0, 1)$ and with $\zeta = 2, 3, 4$, $h_T = h_D = 2^{-11}$ for the reference and the adaptively computed solution.
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Figure: Comparison of the estimated error and actual error. Plots of error w.r. to reference solutions of the quantity $Z'$ w.r. to the cardinality of the index set $\Lambda_N$ (l.) and w.r. to the PDE solves needed (r.) based on the sequence RL with $K = 3$, $\eta \sim \mathcal{N}(0, 1)$ and with $\zeta = 2, 3, 4$, $h_T = h_D = 2^{-11}$ for the reference and the adaptively computed solution.
Numerical Experiments

Model parametric elliptic problem

\[-\text{div}(u\nabla q) = f \quad \text{in} \ D := [0, 1], \ q = 0 \quad \text{in} \ \partial D,\]

with \( f(x) = 100 \cdot x \) and

\[
\ln(u(x, y)) = \sum_{j=1}^{32} \frac{0.1}{(2j)\kappa} \cos(2j\pi x)y_{2j} + \frac{0.1}{(2j - 1)\kappa} \sin((2j - 1)\pi x)y_{2j-1},
\]

where \( y = (y_j)_{j=1,...,64} \) are independently normally distributed, i.e. \( y_j \sim \mathcal{N}(0, 1) \), and \( \kappa = 2, 3, 4 \).

- Finite element method using continuous, piecewise linear ansatz functions in space, backward Euler scheme in time
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Numerical Experiments

Find the unknown data $u$ for given (noisy) data $\delta$,

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- Observation operator $O$ consists of system responses at $K$ observation points in $D$ at
  \begin{align*}
x_j = \frac{j}{2^{N_{K,D}}}, & \quad k = 1, \ldots, 2^{N_{K,D}} - 1, \quad o_k(\cdot) = \delta(\cdot - x_k) \quad \text{with} \quad K = 3, \quad N_{K,D} = 2
\end{align*}
- $G : X \rightarrow \mathbb{R}^K$, with $\phi(u) = G(u)$
- $\eta = (\eta_j)_{j=1,\ldots,K}$ iid with $\eta_j \sim \mathcal{N}(0, 1)$
Numerical Experiments

Quadrature points

- Gauss-Hermite (GH)

\[
W(x) = e^{-x^2}, \quad -\infty < x < \infty
\]

\[
H_{j+1} = 2xH_j - 2jH_{j-1}, \quad H_{-1} = 0, H_0 = 1
\]

with \( n_0 = 1 \) and \( n_k = 2^k + 1 \), for \( k \geq 1 \)
Uncertainty Quantification in Nano Optics

Goal: Quantification of the influence of defects in fabrication process on the optical response of nano structures

- Propagation of plane wave and its interaction with scatterer described by Helmholtz equation (2D).
- Stochastic shape of the scatterer

\[ 0 < \rho_{\text{min}} \leq \rho(\omega, \phi) \leq \rho_{\text{max}}, \quad \omega \in \Omega, \quad \phi \in [0, 2\pi) \]

Collaboration with Ralf Hiptmair, Laura Scarabosio
High Dimensional Initial Value Problem

- Mass action models with uncertain reaction rates
- Biochemical reaction pathways with uncertain reaction rate constants
- Chemical reaction cascades with uncertain reaction rate constants

Goal of computation:
Approximation of system characteristics on the entire, possibly infinite dimensional parameter space

Source: Chen et al., Input-output behavior of ErbB signaling pathways as revealed by a mass action model trained against dynamic data
High Dimensional Initial Value Problem

- Mass action models with uncertain reaction rates
- Biochemical reaction pathways with uncertain reaction rate constants
- Chemical reaction cascades with uncertain reaction rate constants

Source: Chen et al.

Collaboration with the research group of J. Stelling

Source: C. Schillings (SAM - ETHZ)
High Dimensional Initial Value Problem

Given \( x_0(y) \in S \), \( T = [0, 1] \), \( U = [-1, 1]^\mathbb{N} \), find \( X(t, x_0; y) : T \times S \times U \rightarrow S \) such that

\[
\frac{dX}{dt} = f(t, X; y)
\]

\[
= f_0(t, X) + \sum_{j \geq 1} y_j f_j(t, X)
\]

with \( X(0; y) = x_0 \), \( 0 \leq t \leq 1 \), \( \forall y = (y_j)_{j \geq 1} \in U \)

- \( S \) state space (separable and reflexive Banach space)

Affine parameter dependence of the right hand side

Mass action models in computational biology

Stoichiometry with uncertain reaction rate constants
Conclusions and Outlook

- New class of sparse, adaptive quadrature methods for Bayesian inverse problems for a broad class of operator equations
- Dimension-independent convergence rates depending only on the summability of the parametric operator
- Numerical confirmation of the predicted convergence rates
Conclusions and Outlook

- New class of sparse, adaptive quadrature methods for Bayesian inverse problems for a broad class of operator equations
- Dimension-independent convergence rates depending only on the summability of the parametric operator
- Numerical confirmation of the predicted convergence rates

- Gaussian priors and lognormal coefficients
- Adaptive control of the discretization error of the forward problem with respect to the expected significance of its contribution to the Bayesian estimate
- Efficient treatment of large sets of data $\delta$ and small observation noise variance $\Gamma$
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